

Figure S1 The comparison of Lorentzian and MCMC fitting results of simulated data sets under different saturation power.

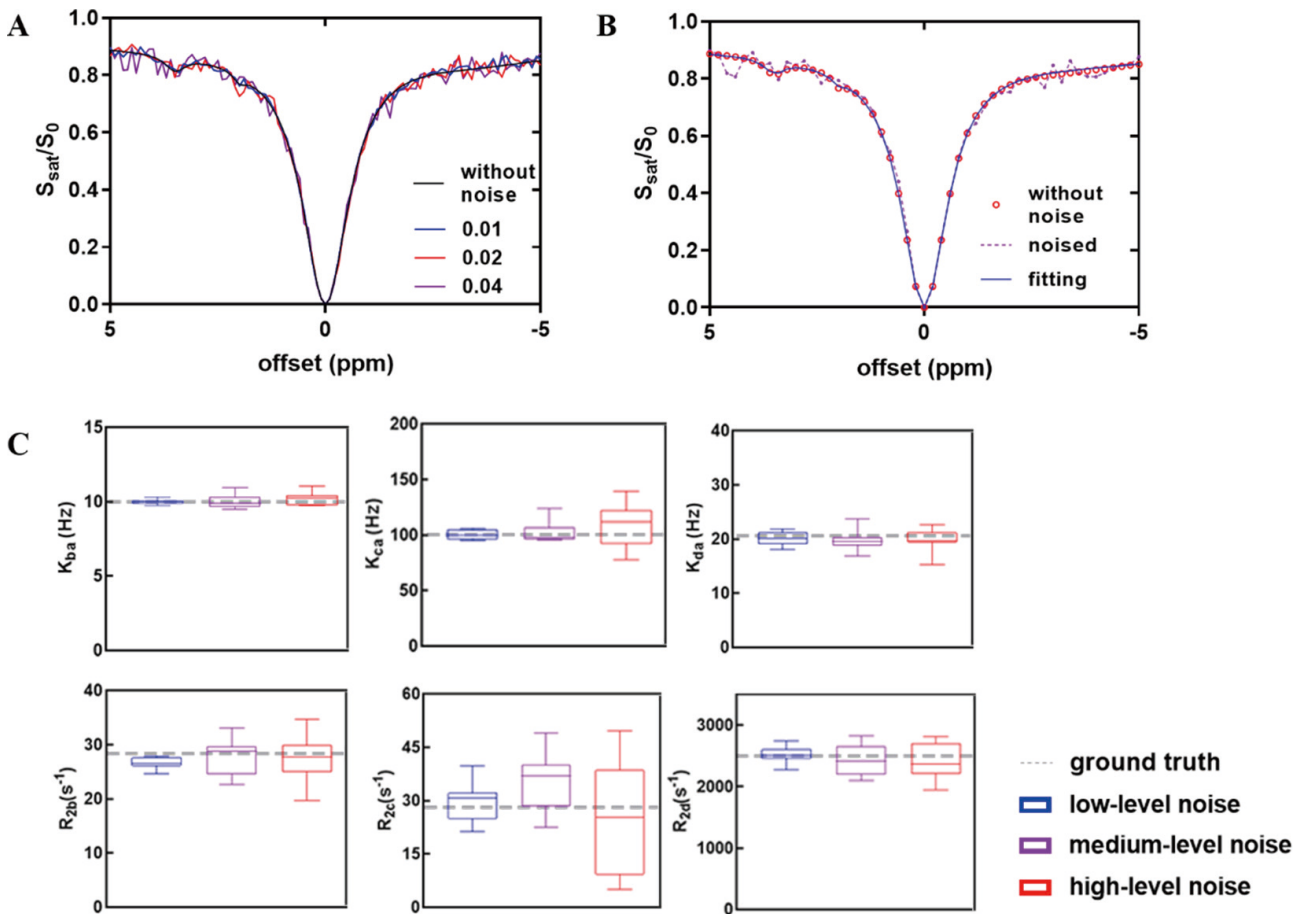
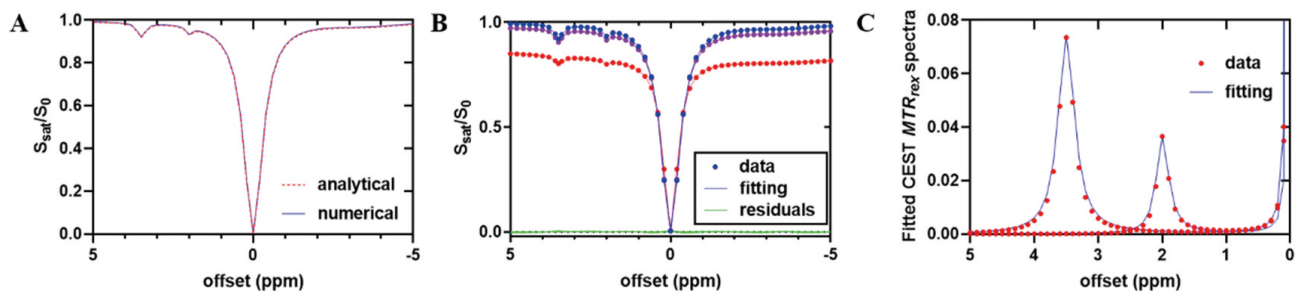


Figure S2 MCMC fitting results of simulated data sets with Gaussian noise added. (A) The simulated Z-spectra with different levels of noise; (B) The Z-spectra fitting with high-level noise; (C) The estimated parameter distributions with different levels of noise.



**Figure S3** MCMC fitting results of simulated data sets obtained with numerical Bloch-McConnell equations for multi-pools models. (A) The comparison between simulations using analytical and numerical solutions; (B) The 5-pools simulation and fitting. Blue circles: low MT concentration cases; Purple circles: medium MT concentration cases; Red circles: high MT concentration cases; (C) The  $MTR_{\text{Rex}}^{\text{Amide}}$  and  $MTR_{\text{Rex}}^{\text{Amine}}$  spectra.